Rainer E Glaser

List of Publications by Year
in descending order

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127 papers	2,915 citations	136940 32 h-index	233409 45 g-index
130 all docs	130 docs citations	130 times ranked	2348 citing authors

#	Article	IF	Citations
1	13C NMR Study of Halogen Bonding of Haloarenes:Â Measurements of Solvent Effects and Theoretical Analysisâ€¡. Journal of the American Chemical Society, 2004, 126, 4412-4419.	13.7	121
2	Planarity ofparaHexaphenyl. Physical Review Letters, 1999, 82, 3625-3628.	7.8	98
3	2,6-Dibenzhydryl-N-(2-phenyliminoacenaphthylenylidene)-4-chloro-aniline nickel dihalides: Synthesis, characterization and ethylene polymerization for polyethylenes with high molecular weights. Journal of Organometallic Chemistry, 2013, 725, 37-45.	1.8	91
4	Semipolar phosphorus-oxygen and phosphorus-carbon bonds. A theoretical study of hypophosphite and related methylenephosphoranes. Journal of the American Chemical Society, 1987, 109, 4184-4188.	13.7	79
5	The effects of the first- and second-row substituents on the structures and energies of PH4X phosphoranes. An ab initio study. Journal of the American Chemical Society, 1991, 113, 55-64.	13.7	74
6	Adenine Synthesis in Interstellar Space: Mechanisms of Prebiotic Pyrimidine-Ring Formation of Monocyclic HCN-Pentamers. Astrobiology, 2007, 7, 455-470.	3.0	65
7	Benzenediazonium Ion. Generality, Consistency, and Preferability of the Electron Density Based Dative Bonding Model. Journal of Organic Chemistry, 1995, 60, 7518-7528.	3.2	64
8	Stereochemistry and Stereoelectronics of Azines. A Solid State Study of Symmetrical, (E,E)-Configured, Para-Substituted (H, F, Cl, Br, CN) Acetophenone Azines. Journal of Organic Chemistry, 1994, 59, 4336-4340.	3.2	63
9	Pushâ€“pull substitution versus intrinsic or packing related Nâ€“N gauche preferences in azines. Synthesis, crystal structures and packing of asymmetrical acetophenone azines. Journal of the Chemical Society Perkin Transactions II, 1995, , 2311-2317.	0.9	60
10	Charge transfers and polarizations in bonds to silicon. Organosilanes and the SN2(Si) reaction of silane with fluoride. An ab initio study. Journal of the American Chemical Society, 1989, 111, 3111-3117.	13.7	56
11	Aspirin. An ab Initio Quantum-Mechanical Study of Conformational Preferences and of Neighboring Group Interactions. Journal of Organic Chemistry, 2001, 66, 771-779.	3.2	54
12	Ab Initio Study of the SN1Ar and SN2Ar Reactions of Benzenediazonium Ion with Water. On the Conception of â€œUnimolecular Dediazoniationâ€•in Solvolysis Reactions. Journal of the American Chemical Society, 2004, 126, 10632-10639.	13.7	50
13	The Azine Bridge as a Conjugation Stopper:Â An NMR Spectroscopic Study of Electron Delocalization in Acetophenone Azinesâ€. Journal of Organic Chemistry, 2002, 67, 1441-1447.	3.2	49
14	Synergism of Catalysis and Reaction Center Rehybridization. A Novel Mode of Catalysis in the Hydrolysis of Carbon Dioxide. Journal of Physical Chemistry A, 2003, 107, 6814-6818.	2.5	48
15	Conjugation in azines. Stereochemical analysis of benzoylformate azines in the solid state, in solution, and in the gas phase. Journal of Organic Chemistry, 1993, 58, 7446-7455.	3.2	47
16	THE CARRIERS OF THE INTERSTELLAR UNIDENTIFIED INFRARED EMISSION FEATURES: CONSTRAINTS FROM THE INTERSTELLAR C-H STRETCHING FEATURES AT 3.2-3.5 Î¼m. Astrophysical Journal, 2013, 776, 110.	4.5	44
17	Tuning Intermolecular Interactions:â€‰ A Study of the Structural and Vibrational Properties of p-Hexaphenyl under Pressure. Journal of Physical Chemistry A, 2001, 105, 6203-6211.	2.5	43
18	Thermochemistry of the Initial Steps of Methylaluminoxane Formation. Aluminoxanes and Cycloaluminoxanes by Methane Elimination from Dimethylaluminum Hydroxide and Its Dimeric Aggregates. Journal of the American Chemical Society, 2011, 133, 13323-13336.	13.7	42

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19	Ïƒ-Dative and Ï€-Backdative Phenyl Cationâ^'Dinitrogen Interactions and Opposing Sign Reaction Constants in Dual Substituent Parameter Relationsâ€. Journal of Organic Chemistry, 1999, 64, 902-913.	3.2	41
20	Configurational and conformational preferences in oximes and oxime carbanions. Ab initio study of the syn effect in reactions of oxyimine enolate equivalents. Journal of the American Chemical Society, 1989, 111, 7340-7348.	13.7	40
21	Organic Chemistry Online: Building Collaborative Learning Communities through Electronic Communication Tools. Journal of Chemical Education, 1999, 76, 699.	2.3	40
22	Polymorphism and C?N?N?C Conformational Isomers of Azines: X-ray Crystal and Ab Initio Structures of Two Rotational Isomers of Methyl (para-Tolyl) Ketone Azine. Angewandte Chemie International Edition in English, 1994, 33, 1081-1084.	4.4	39
23	Asymmetrization effects on structures and populations of the ground state of dipolar donor-acceptor-substituted molecular organic NLO materials. Journal of Computational Chemistry, 1998, 19, 1130-1140.	3.3	39
24	Theoretical Studies of DNA Base Deamination. 2. Ab Initio Study of DNA Base Diazonium Ions and of Their Linear, Unimolecular Dediazoniation Pathsâ€,Â§. Journal of the American Chemical Society, 1999, 121, 6108-6119.	13.7	39
25	Synergism of Catalysis and Reaction Center Rehybridization. An ab Initio Study of the Hydrolysis of the Parent Carbodiimide. Journal of the American Chemical Society, 1998, 120, 8541-8542.	13.7	37
26	Chloroyttrium 2-(1-(Arylimino)alkyl)quinolin-8-olate Complexes: Synthesis, Characterization, and Catalysis of the Ring-Opening Polymerization of Îµ-Caprolactone. Organometallics, 2012, 31, 8178-8188.	2.3	37
27	Incipient nucleophilic attack as a probe for the electronic structure of diazonium ions. An analysis of neighboring-group interactions in .beta.-(carboxyvinyl)diazonium ions. Journal of Organic Chemistry, 1992, 57, 215-228.	3.2	35
28	Pyrimidine Ring Opening in the Unimolecular Dediazoniation of Guanine Diazonium Ion. An Ab Initio Theoretical Study of the Mechanism of Nitrosative Guanosine Deamination. Journal of the American Chemical Society, 1996, 118, 10942-10943.	13.7	35
29	Importance of the anisotropy of atoms in molecules for the representation of electron density distributions with Lewis structures. A case study of aliphatic diazonium ions. Journal of the American Chemical Society, 1993, 115, 2340-2347.	13.7	34
30	Single- and Double-Proton-Transfer in the Aggregate between Cytosine and Guaninediazonium Ionâ€,Â§. Organic Letters, 1999, 1, 273-276.	4.6	34
31	Ab Initio and Crystal Structures of (E,E)-1,4-Diphenylbutadiene:â€‰ A New Type of Areneâ^'Arene Double T-Contact and an Interesting Interlayer Cooperation Involving Diastereoisomeric Contacts. Crystal Growth and Design, 2003, 3, 291-300.	3.0	34
32	Analysis of the remarkable difference in the stabilities of methyl- and ethyldiazonium ions. Journal of the American Chemical Society, 1991, 113, 1109-1120.	13.7	33
33	Comparative analysis of crystal structures of E,E-configured para-substituted acetophenone azines with halogen, oxygen, nitrogen and carbon functional groups. Journal of the Chemical Society Perkin Transactions II, 1995, , 1449.	0.9	32
34	The carriers of the unidentified infrared emission features: Clues from polycyclic aromatic hydrocarbons with aliphatic sidegroups. New Astronomy Reviews, 2017, 77, 1-22.	12.8	31
35	Polar Order by Rational Design:â€‰ Crystal Engineering with Parallel Beloamphiphile Monolayers. Accounts of Chemical Research, 2007, 40, 9-17.	15.6	30
36	Crystal Potential Formula for the Calculation of Crystal Lattice Sums. Journal of Physical Chemistry B, 1998, 102, 4257-4260.	2.6	29

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37	Origin of the Stabilization of Vinyldiazonium Ions byÎ²-Substitution; First Crystal Structure of an Aliphatic Diazonium Ion:Î²,Î²-Diethoxyethene-diazonium Hexachloroantimonate. Angewandte Chemie International Edition in English, 1992, 31, 740-743.	4.4	26
38	Electron-Density Relaxation and Oppositely Signed Reaction Constants in Dual Substituent Parameter Relationships in Dediazoniation Reactions. Angewandte Chemie International Edition in English, 1997, 36, 2210-2213.	4.4	26
39	Cytosine Catalysis of Nitrosative Guanine Deamination and Interstrand Cross-Link Formation. Journal of the American Chemical Society, 2005, 127, 7346-7358.	13.7	26
40	Theoretical study of structures and relative energies of isomeric metalated acetaldoximes, models for metalated oxime ethers. Journal of the American Chemical Society, 1987, 109, 1258-1260.	13.7	25
41	The supramolecular architecture of 4-aminoacetophenone (1-(4-fluorophenyl)ethylidene)hydrazone hydrate. Double T-contacts and extremely low-density water layers in a mixed azine. Canadian Journal of Chemistry, 1998, 76, 1371-1378.	1.1	25
42	Interpretation of neighboring group interactions in crystal structures. A solid state and quantum-chemical study of "incipient nucleophilic attack" in 2-diazonium benzoic acid and its benzoate. Canadian Journal of Chemistry, 1996, 74, 1200-1214.	1.1	24
43	Structures of nitroso- and nitroguanidine X-ray crystallography and computational analysis. Journal of Chemical Crystallography, 2005, 35, 317-325.	1.1	23
44	Electronic Excitations in Homopolyatomic Bismuth Cations: Spectroscopic Measurements in Molten Salts and an ab initio CI-Singles Study. Chemistry - A European Journal, 2000, 6, 1078-1086.	3.3	22
45	On the Reaction Mechanism of Tirapazamine Reduction Chemistry: Unimolecular Nâ€“OH Homolysis, Stepwise Dehydration, or Triazene Ring-Opening. Chemical Research in Toxicology, 2012, 25, 634-645.	3.3	22
46	A higher level ab initio quantum-mechanical study of the quadrupole moment tensor components of carbon dioxide. Journal of Molecular Structure, 2000, 556, 131-141.	3.6	21
47	Synergism of Catalysis and Reaction Center Rehybridization in Nucleophilic Additions to Cumulenes: The One-, Two- and Three-Water Hydrolyses of Carbodiimide and Methyleneimine Part 5 in the Series â€œNucleophilic Additions to Heterocumulenes.â€•For Part 4, see ref. [19].. Chemistry - A European Journal, 2002, 8, 1934.	3.3	21
48	Dynamical Approach to Multiequilibria Problems for Mixtures of Acids and Their Conjugated Bases. Journal of Chemical Education, 2014, 91, 1009-1016.	2.3	21
49	5-Cyanoimino-4-oxomethylene-4,5-dihydroimidazole and Nitrosative Guanine Deamination. A Theoretical Study of Geometries, Electronic Structures, and N-Protonationâ€. Journal of Organic Chemistry, 2003, 68, 9882-9892.	3.2	20
50	Nitrosative Adenine Deamination:â€‰ Facile Pyrimidine Ring-Opening in the Dediazoniation of Adeninediazonium Ion. Organic Letters, 2003, 5, 4077-4080.	4.6	20
51	Chemistry Is in the News: Taxonomy of authentic news mediaâ€based learning activities1. International Journal of Science Education, 2005, 27, 1083-1098.	1.9	20
52	Coordinate Covalent C â†’ B Bonding in Phenylborates and Latent Formation of Phenyl Anions from Phenylboronic Acidâ€. Journal of Physical Chemistry A, 2006, 110, 1295-1304.	2.5	20
53	Chemistry Is in the News: Assessment of Student Attitudes toward Authentic News Media-Based Learning Activities. Journal of Chemical Education, 2006, 83, 662.	2.3	20
54	THE Câ€“H STRETCHING FEATURES AT 3.2â€“3.5 Î¼m OF POLYCYCLIC AROMATIC HYDROCARBONS WITH ALIPHATIC SIDEGROUPS. Astrophysical Journal, 2016, 825, 22.	4.5	20

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55	Stereochemistry of metalated aldimines. 1. An ab initio study of the potential energy surfaces of isolated acetaldimine anions, their monomeric lithium and sodium ion pairs, and mechanistic consequences. Journal of Organic Chemistry, 1991, 56, 6612-6624.	3.2	19
56	Stereochemistry and Stereoelectronics of Azines. 13. Conformational Effects on the Quadrupolarity of Azines. An Ab Initio Quantum-Mechanical Study of a Lateral Synthon. Journal of Molecular Modeling, 2000, 6, 86-98.	1.8	19
57	5-Cyanoimino-4-oxomethylene-4,5-dihydroimidazole and 5-Cyanoamino-4-imidazolecarboxylic Acid Intermediates in Nitrosative Guanosine Deamination:â€‰ Evidence from 18O-Labeling Experiments. Journal of the American Chemical Society, 2004, 126, 9960-9969.	13.7	19
58	Nitrosation Chemistry of Pyrroline, 2-Imidazoline, and 2-Oxazoline:Â Theoretical Curtinâ^'Hammett Analysis of Retro-Ene and Solvent-Assisted Câ^'X Cleavage Reactions of Î±-Hydroxy-N-Nitrosamines. Journal of Organic Chemistry, 2005, 70, 6790-6801.	3.2	19
59	4-Chloroacetophenone [1-(4-methoxyphenyl)ethylidene]hydrazone. Acta Crystallographica Section C: Crystal Structure Communications, 2000, 56, 393-396.	0.4	18
60	Demonstration of an Alternative Mechanism forG-to-GCross-Link Formation. Journal of the American Chemical Society, 2005, 127, 880-887.	13.7	18
61	Spin Polarization versus Spin Delocalization. Topological Electron and Spin Density Analysis of the Rotational Automerization of Allyl Radical Including Electron Correlation Effects1. The Journal of Physical Chemistry, 1994, 98, 11379-11393.	2.9	17
62	Title is missing!. Journal of Chemical Crystallography, 2000, 30, 489-496.	1.1	17
63	Polarizabilities of Carbon Dioxide and Carbodiimide. Assessment of Theoretical Model Dependencies on Dipole Polarizabilities and Dipole Polarizability Anisotropiesâ€. Journal of Physical Chemistry A, 2000, 104, 11355-11361.	2.5	17
64	Perfect polar stacking of parallel beloamphiphile layers. Synthesis, structure and solid-state optical properties of the unsymmetrical acetophenone azine DCA. Dalton Transactions, 2006, , 2891.	3.3	17
65	Stabilities and Spin Distributions of Benzannulated Benzyl Radicals. Journal of Chemical Theory and Computation, 2007, 3, 1091-1099.	5.3	17
66	Tris(chalkogeno)carbeniumâ€ionen [C(XR)₃]⁺(X = O, S, Se, Te): ein experimenteller und quantenchemischer Vergleich. Angewandte Chemie, 1996, 108, 317-320.	2.0	16
67	5-Cyanoamino-4-imidazolecarboxamide and Nitrosative Guanine Deamination:Â Experimental Evidence for Pyrimidine Ring-Opening during Deamination. Journal of the American Chemical Society, 2004, 126, 2274-2275.	13.7	16
68	Near-Silence of Isothiocyanate Carbon in 13C NMR Spectra: A Case Study of Allyl Isothiocyanate. Journal of Organic Chemistry, 2015, 80, 4360-4369.	3.2	16
69	Diazonium ions. Topological electron density analysis of cyclopropeniumyldiazonium dications and of their stability toward dediazoniation. Journal of Computational Chemistry, 1990, 11, 663-679.	3.3	15
70	Stereochemistry of metalated aldimines. 2. A theoretical study of dimeric ion-pair aggregates of isomeric lithioacetaldimines and of their kinetically controlled reaction with formaldehyde. Journal of Organic Chemistry, 1991, 56, 6625-6637.	3.2	15
71	Heterosubstituted diazonium ions FNN+, HONN+, and H2NNN+. Automerization, dediazoniation, and deprotonation. The Journal of Physical Chemistry, 1991, 95, 7682-7693.	2.9	15
72	Electron and spin density analysis of spin-projected unrestricted Hartree-Fock density matrixes of radicals. The Journal of Physical Chemistry, 1993, 97, 3188-3198.	2.9	15

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73	Nitrosative Guanine Deamination:Â Ab Initio Study of Deglycation ofN-Protonated 5-Cyanoimino-4-oxomethylene-4,5-dihydroimidazoles. Chemical Research in Toxicology, 2004, 17, 1157-1169.	3.3	15
74	Multifurcated halogen bonding involving Phâ€“Clâ‹¯Hâ€“CPhî€Nâ€“Râ€² interactions and its relation to idioteloamphiphile layer architecture. CrystEngComm, 2006, 8, 372-376.	2.6	15
75	Theoretical Study of the Quadrupolarity of Carbodiimideâ€. Journal of Physical Chemistry A, 2002, 106, 7950-7957.	2.5	14
76	Nitrosative Cytosine Deamination. An Exploration of the Chemistry Emanating from Deamination with Pyrimidine Ring-Opening. Chemical Research in Toxicology, 2005, 18, 1211-1218.	3.3	14
77	Ammonia elimination from protonated nucleobases and related synthetic substrates. Journal of the American Society for Mass Spectrometry, 2007, 18, 2040-2057.	2.8	14
78	The Cationâ€Đinitrogen Interaction in the â€œBenzyldiazonium ionâ€• Preferential Electrostatic Complex Formation and Dinitrogen Catalysis of Benzyl Cation Rotational Automerization. Chemistry - A European Journal, 1997, 3, 1244-1253.	3.3	13
79	What's in a name? Noncovalent Arâ€“ClÂ·(Hâ€“Arâ€²)ninteractions and terminology based on structure and nature of the bonding. CrystEngComm, 2006, 8, 948-951.	2.6	13
80	Chemistry Is in the News: assessing intraâ€group peer review. Assessment and Evaluation in Higher Education, 2010, 35, 381-402.	5.6	13
81	3-Methylcarboxy-1H-indazole. Theoretical study of its formation via intramolecular aliphatic diazonium coupling and x-ray crystal structure. Journal of Physical Organic Chemistry, 1993, 6, 201-214.	1.9	12
82	The crystal structure of 4-iodoacetophenone azine. Journal of Chemical Crystallography, 1999, 29, 1043-1048.	1.1	12
83	Amino Effect on the Protonation of Î²-Aminoacrylonitrile. Chemical Research in Toxicology, 2005, 18, 111-114.	3.3	12
84	Aluminum alkoxyâ€catalyzed biomass conversion of glucose to 5â€hydroxymethylfurfural: Mechanistic study of the cooperative bifunctional catalysis. Journal of Computational Chemistry, 2019, 40, 1599-1608.	3.3	12
85	Conformational Preferences and Pathways for Enantiomerization and Diastereomerization of Benzyl Alcohol. Data Mining and ab Initio Quantum-Mechanical Study. Journal of Organic Chemistry, 2000, 65, 755-766.	3.2	11
86	Learning To Read Spectra: Teaching Decomposition with Excel in a Scientific Writing Course. Journal of Chemical Education, 2018, 95, 476-481.	2.3	11
87	Simultaneous Determination of All Species Concentrations in Multiequilibria for Aqueous Solutions of Dihydrogen Phosphate Considering Debyeâ€“HÃ¼ckel Theory. Journal of Chemical & Engineering Data, 2018, 63, 2151-2161.	1.9	11
88	Superhydrogenated Polycyclic Aromatic Hydrocarbon Molecules: Vibrational Spectra in the Infrared. Astrophysical Journal, Supplement Series, 2020, 247, 1.	7.7	11
89	Dynamic aspects of the stereochemistry of metalated oxime ethers. An ab initio study of the pathways for coordination-isomerization, for syn/anti isomerization, and for racemization of the lithium ion pairs from acetaldoxime. Journal of the American Chemical Society, 1989, 111, 8799-8809.	13.7	10
90	Electron and Spin-Density Analysis of Tirapazamine Reduction Chemistry. Chemical Research in Toxicology, 2012, 25, 620-633.	3.3	10

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91	Disproportionation of Bromous Acid HOBrO by Direct O-Transfer and via Anhydrides O(BrO)₂ and BrOâ€“BrO₂. An Ab Initio Study of the Mechanism of a Key Step of the Belousovâ€“Zhabotinsky Oscillating Reaction. Journal of Physical Chemistry A, 2012, 116, 8352-8365.	2.5	10
92	Crystal Structure of the Explosive Parent Benzyne Precursor: 2â€Ð iazoniobenzenecarboxylate Hydrate. Chemische Berichte, 1993, 126, 243-249.	0.2	9
93	Inductive and Conjugative Sâ†'C Polarizations in â€œTrithiocarbenium Ionsâ€•[C(SH)3]+ and [C(SH)3]â€¢,2+. Potential Energy Surface Analysis, Electronic Structure Motif, and Spin Density Distribution. Journal of the American Chemical Society, 1996, 118, 11617-11628.	13.7	9
94	Elektronendichteverschiebungen und Reaktionskonstanten mit entgegengesetzten Vorzeichen bei der Analyse von Dediazonierungsreaktionen mit Hilfe dualer Substituentenparameter. Angewandte Chemie, 1997, 109, 2324-2328.	2.0	9
95	Dynamical Approach to Multi-Equilibria Problems Considering the Debyeâ€“HÃ¼ckel Theory of Electrolyte Solutions: Concentration Quotients as a Function of Ionic Strength. Journal of Solution Chemistry, 2017, 46, 643-662.	1.2	9
96	Deuterated Polycyclic Aromatic Hydrocarbons in the Interstellar Medium: The Câ€“D Band Strengths of Monodeuterated Species. Astrophysical Journal, Supplement Series, 2020, 251, 12.	7.7	8
97	Dipole Parallel Alignment in the Crystal Structure of a Polar Biphenyl:â€‰ 4â€˜-Acetyl-4-Methoxybiphenyl (AMB)â€. Crystal Growth and Design, 2006, 6, 235-240.	3.0	7
98	Asymmetry in the N-Inversion of Heteroarene Imines: Pyrimidin-4(3H)-Imine, Pyridin-2(1H)-Imine, and 1H-Purine-6(9H)-Imine. Journal of Organic Chemistry, 2010, 75, 1132-1142.	3.2	7
99	Asymmetric ImineN-Inversion in 3-Methyl-4-pyrimidinimine. Molecular Dipole Analysis of Solvation Effects. Journal of Organic Chemistry, 2011, 76, 3987-3996.	3.2	7
100	Mechanistic Models for LAH Reductions of Acetonitrile and Malononitrile. Aggregation Effects of Li⁺ and AlH₃ on Imideâ€“Enamide Equilibria. Journal of Organic Chemistry, 2013, 78, 1113-1126.	3.2	7
101	Enhanced piezoresponse and nonlinear optical properties of fluorinated self-assembled peptide nanotubes. AIP Advances, 2019, 9, 115202.	1.3	7
102	Software for the Synergistic Integration of Science with ICT Education. Journal of Information Technology Education:Research, 0, 3, 325-339.	0.0	7
103	Ab initio study of the regiochemistry of dimetalated oximes. The importance of triple ions in isomeric lithium and sodium ion pairs of the acetaldoxime dianion. Journal of Organic Chemistry, 1989, 54, 5491-5502.	3.2	6
104	The Heterolytic Dissociation of Neutral and Protonated Nitrous Acid. Journal of Physical Chemistry A, 2003, 107, 11112-11119.	2.5	6
105	Challenges of Globalization and Successful Adaptation Strategies in Implementing a â€œScientific Writing and Authoringâ€•Course in China. Journal of Chemical Education, 2018, 95, 2155-2163.	2.3	6
106	Deuterated Polycyclic Aromatic Hydrocarbons in the Interstellar Medium: The Câ€“D Band Strengths of Multideuterated Species. Astrophysical Journal, Supplement Series, 2021, 255, 23.	7.7	6
107	Lattice sum calculations for 1/rp interactions via multipole expansions and Euler summation. Journal of Computational Chemistry, 2001, 22, 208-215.	3.3	5
108	Electronic Structures and Spin Topologies of Î³-Picoliniumyl Radicals. A Study of the Homolysis of N-Methyl-Î³-picolinium and of Benzo-, Dibenzo-, and Naphthoannulated Analogs. Journal of Physical Chemistry A, 2008, 112, 4800-4814.	2.5	5

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109	Biomimetic Approaches to Reversible CO2 Capture from Air. N-Methylcarbaminic Acid Formation in Rubisco-Inspired Models. , 2013, , 501-534.		5
110	Effects of electron correlation and spin projection on rotational barriers of trithiocarbenium ion [C(SH)3]+ and Radical Dication [C(SH)3]?,2+. Journal of Computational Chemistry, 1997, 18, 1023-1035.	3.3	4
111	Chemical carcinogens in non-enzymatic cytosine deamination: 3-isocyanatoacrylonitrile. Journal of Molecular Modeling, 2006, 12, 731-737.	1.8	4
112	Iodine Bonding Stabilizes Iodomethane in MIDAS Pesticide. Theoretical Study of Intermolecular Interactions between Iodomethane and Chloropicrin. Journal of Agricultural and Food Chemistry, 2012, 60, 1776-1787.	5.2	4
113	Thermochemistry of a Biomimetic and Rubisco-Inspired CO2 Capture System from Air. Journal of Carbon Research, 2016, 2, 18.	2.7	4
114	Measurements and Simulations of the Acidity Dependence of the Kinetics of the Iron-Catalyzed Belousovâ€“Zhabotinsky Reaction: Proton-Catalysis in the Electron Transfer Reaction Involving the [Fe(phen)₃]³⁺ Species. Journal of Physical Chemistry A, 2018, 122, 6183-6195.	2.5	4
115	Potential Energy Surface and Electron Density Analysis of Phosphorus Analogues of Aromatic and Aliphatic Diazonium Ions. Phosphorus, Sulfur and Silicon and the Related Elements, 1993, 77, 73-76.	1.6	3
116	Arene-Arene Double T-Contacts: Lateral Synthons in the Engineering of Highly Anisotropic Organic Molecular Crystals. ACS Symposium Series, 2001, , 97-111.	0.5	3
117	Embedding 1,6-Diphenyl-1,2-Dihydronaphthalene (DHN) in 1,4-Distyrylbenzene (DSB):â€‰Areneâ‹¯Arene Interactions in a â€œCrossed Bis-Diareneâ€• Crystal Growth and Design, 2006, 6, 1014-1021.	3.0	3
118	RuBisCO-Inspired Biomimetic Approaches to Reversible CO₂Capture from Air. ACS Symposium Series, 2015, , 265-293.	0.5	3
119	Computational Investigation of the Thermochemistry of the CO₂ Capture Reaction by Ethylamine, Propylamine, and Butylamine in Aqueous Solution Considering the Full Conformational Space via Boltzmann Statistics. Journal of Physical Chemistry A, 2021, 125, 9578-9593.	2.5	3
120	Transition Metal-Catalyzed and MAO-Assisted Olefin Polymerization; Cyclic Isomers of Sinnâ€™s Dimer Are Excellent Ligands in Iron Complexes and Great Methylating Reagents. Catalysts, 2022, 12, 312.	3.5	3
121	Polymorphie und Cï£¾Nï£¿Nï£¾Câ€Konformationsâ€isomerie in Azinen: Strukturen zweier Rotationsisomere von Methyl(paraâ€tolyl)ketonazin im Kristall und mit abâ€initioâ€Methoden berechnet. Angewandte Chemie, 1994, 106, 1150-1152.	2.0	2
122	ADDITIVITY SCHEMES IN CONFORMATIONAL ANALYSIS: CONCEPT AND DEMONSTRATION. Journal of Theoretical and Computational Chemistry, 2005, 04, 373-381.	1.8	2
123	Electronic Structures and Spin Density Distributions of BrO₂ and (HO)₂BrO Radicals. Mechanisms for Avoidance of Hypervalency and for Spin Delocalization and Spin Polarization. Inorganic Chemistry, 2013, 52, 11806-11820.	4.0	2
124	Video-Based Kinetic Analysis of Period Variations and Oscillation Patterns in the Ce/Fe-Catalyzed Four-Color Belousovâ€“Zhabotinsky Oscillating Reaction. ACS Symposium Series, 2019, , 251-270.	0.5	1
125	Video colorimetry of single-chromophore systems based on vector analysis in the 3D color space: Unexpected hysteresis loops in oscillating chemical reactions. Talanta, 2020, 220, 121303.	5.5	1
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127	Chemical carcinogens in non-enzymatic cytosine deamination: 3-isocyanatoacrylonitrile. , 2006, , 731-737.		0